GIAN-CARLO ROTA, *Editor*

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Volume 5

Section: Statistical Mechanics

Giovanni Gallavotti, *Section Editor*

Thermodynamic Formalism
The Mathematical Structures of Classical Equilibrium Statistical Mechanics

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With a Foreword by
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Editor's Statement

A large body of mathematics consists of facts that can be presented and described much like any other natural phenomenon. These facts, at times explicitly brought out as theorems, at other times concealed within a proof, make up most of the applications of mathematics, and are the most likely to survive changes of style and of interest.

This ENCYCLOPEDIA will attempt to present the factual body of all mathematics. Clarity of exposition, accessibility to the non-specialist, and a thorough bibliography are required of each author. Volumes will appear in no particular order, but will be organized into sections, each one comprising a recognizable branch of present-day mathematics. Numbers of volumes and sections will be reconsidered as times and needs change.

It is hoped that this enterprise will make mathematics more widely used where it is needed, and more accessible in fields in which it can be applied but where it has not yet penetrated because of insufficient information.

GIAN-CARLO ROTA

Section Editor's Foreword

Thermodynamics is still, as it always was, at the center of physics, the standard-bearer of successful science. As happens with many a theory, rich in applications, its foundations have been murky from the start and have provided a traditional challenge on which physicists and mathematicians alike have tested their latest skills.

Ruelle's book is perhaps the first entirely rigorous account of the foundations of thermodynamics. It makes heavier demands on the reader's mathematical background than any volume published so far. It is hoped that ancillary volumes in time will be published which will ease the ascent onto this beautiful and deep theory; at present, much of the background material can be gleaned from standard texts in mathematical analysis. In any case, the timeliness of the content shall be ample reward for the austerity of the text.

GIOVANNI GALLAVOTTI
General Editor, Section on Statistical Mechanics
and
GIAN-CARLO ROTA

Preface

The present monograph is based on lectures given in the mathematics departments of Berkeley (1973) and of Orsay (1974–75). My aim has been to describe the mathematical structures underlying the thermodynamic formalism of equilibrium statistical mechanics, in the simplest case of classical lattice spin systems.

The thermodynamic formalism has its origins in physics, but it has now invaded topological dynamics and differentiable dynamical systems, with applications to questions as diverse as the study of invariant measures for an Anosov diffeomorphism (Sinai [3]), or the meromorphy of Selberg's zeta function (Ruelle [7]). The present text is an introduction to such questions, as well as to more traditional problems of statistical mechanics, like that of phase transitions. I have developed the general theory—which has considerable unity—in some detail. I have however left aside particular techniques (like that of correlation inequalities) which are important in discussing examples of phase transitions, but should be the object of a special study.

Statistical mechanics extends to systems vastly more general than the classical lattice spin systems discussed here (in particular to quantum systems). One can therefore predict that the theory discussed in this monograph will extend to vastly more general mathematical setups (in particular to non-commutative situations). I hope that the present text may contribute some inspiration to the construction of the more general theories, as well as clarifying the conceptual structure of the existing formalism.

DAVID RUELLE

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CHAPTER 0

Introduction

0.1 Generalities

The formalism of equilibrium statistical mechanics—which we shall call *thermodynamic formalism*—has been developed since G. W. Gibbs to describe the properties of certain physical systems. These are systems consisting of a large number of subunits (typically 10^{27}) like the molecules of one liter of air or water. While the physical justification of the thermodynamic formalism remains quite insufficient, this formalism has proved remarkably successful at explaining facts.

In recent years it has become clear that, underlying the thermodynamic formalism, there are mathematical structures of great interest: the formalism hints at the good theorems, and to some extent at their proofs. Outside of statistical mechanics proper, the thermodynamic formalism and its mathematical methods have now been used extensively in *constructive quantum field theory** and in the study of certain *differentiable dynamical systems* (notably Anosov diffeomorphisms and flows). In both cases the relation is at an abstract mathematical level, and fairly inobvious at first sight. It is evident that the study of the physical world is a powerful source of inspiration for mathematics. That this inspiration can act in such a detailed manner is a more remarkable fact, which the reader will interpret according to his own philosophy.

The main physical problem which equilibrium statistical mechanics tries to clarify is that of phase transitions. When the temperature of water is lowered, why do its properties change first smoothly, then suddenly as the freezing point is reached? While we have some general ideas about this, and many special results, a conceptual understanding is still missing.† The

*See for instance Velo and Wightman [1].

†At a more phenomenological level, a good deal is known about phase transitions and much attention has been devoted to critical points and "critical phenomena"; the latter remain however for the moment inaccessible to rigorous investigations.

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mathematical investigation of the thermodynamic formalism is in fact not completed; the theory is a young one, with emphasis still more on imagination than on technical difficulties. This situation is reminiscent of preclassic art forms, where inspiration has not been castrated by the necessity to conform to standard technical patterns. We hope that some of this juvenile freshness of the subject will remain in the present monograph!

The physical systems to which the thermodynamic formalism applies are idealized to be actually infinite, i.e. to fill $\mathbf{R}^\nu$ (where $\nu=3$ in the usual world). This idealization is necessary because only infinite systems exhibit sharp phase transitions. Much of the thermodynamic formalism is concerned with the study of *states* of infinite systems.

For *classical systems* the states are probability measures on an appropriate space of infinite configurations; such states can also be viewed as linear functionals on an abelian algebra (an algebra of continuous functions in the case of Radon measures). For *quantum systems* the states are "expectation value" linear functionals on non-abelian algebras. Due to their greater simplicity, classical systems have been studied more than quantum systems. In fact attention has concentrated on the simplest systems, the *classical lattice systems* where $\mathbf{R}^\nu$ is replaced by $\mathbf{Z}^\nu$ (a ν-dimensional crystal lattice). For such systems the configuration space is a subset Ω of $\prod_{x\in\mathbf{Z}^\nu}\Omega_x$ (where Ω_x is for instance the set of possible "spin values" or "occupation numbers" at the lattice site x). We shall assume that Ω_x is finite. Due to the group invariance (under $\mathbf{Z}^\nu$ or $\mathbf{R}^\nu$) the study of states of infinite systems is closely related to ergodic theory. There are however other parts of the thermodynamic formalism concerned with quite different questions (like analyticity problems).

The present monograph addresses itself to mathematicians. Its aim is to give an account of part of the thermodynamic formalism, and of the corresponding structures and methods. We have restricted ourselves to classical lattice systems. The thermodynamic formalism extends to many other classes of systems, but the theory as it exists now for those systems is less complete, more singular, and filled with technical difficulties. The formalism which we shall describe would not apply directly to the problems of constructive quantum field theory, but it is appropriate to the discussion of Anosov diffeomorphisms and related dynamical systems.

The mathematics underlying the thermodynamic formalism consists of general methods and special techniques. We have restricted ourselves in this monograph to the general methods; we hope that a complement on special techniques will be published later. As a rough rule, we have decided that a result was not "general" if it required that the configuration space of the system factorize completely in the form $\Omega=\prod\Omega_x$, where Ω_x is the finite set of "spin values" at the lattice site x. The body of general methods thus defined has considerable unity. As for the special techniques, let us mention the correlation inequalities, the method of integral equations, the

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Lee-Yang circle theorem, and the Peierls argument. These techniques look somewhat specialized from the general point of view taken in this monograph, but are often extremely elegant. They provide, in special situations, a variety of detailed results of great interest for physics.

0.2 Description of the Thermodynamic Formalism

The contents of this section are not logically required for later chapters. We describe here, for purposes of motivation and orientation, some of the ideas and results of the thermodynamic formalism.* The reader may go over this material rapidly, or skip it entirely.

I. Finite systems

Let Ω be a non-empty finite set. Given a probability measure σ on Ω we define its *entropy*

$$S(\sigma)=-\sum_{\xi\in\Omega}\sigma\{\xi\}\log\sigma\{\xi\},$$

where it is understood that $t\log t=0$ if $t=0$. Given a function $U:\Omega\to\mathbf{R}$, we define a real number Z called the *partition function* and a probability measure ρ on Ω called the *Gibbs ensemble* by

$$Z=\sum_{\xi\in\Omega}\exp[-U(\xi)],$$
$$\rho\{\xi\}=Z^{-1}\exp[-U(\xi)]. \tag{0.1}$$

Proposition (Variational principle). *The maximum of the expression*†

$$S(\sigma)-\sigma(U)$$

over all probability measures σ on Ω is $\log Z$, and is reached precisely for $\sigma=\rho$.

For physical applications, Ω is interpreted as the space of configurations of a finite system. One writes $U=\beta E$, where $E(\xi)$ is the energy of the configuration ξ, and $\beta=1/kT$, where T is the absolute temperature and k is a factor known as Boltzmann's constant. The problem of why the Gibbs ensemble describes thermal equilibrium (at least for "large systems") when

*We follow in part the Séminaire Bourbaki, exposé 480.
†We write $\sigma(U)=\Sigma_\xi\sigma\{\xi\}U(\xi)$ or more generally $\sigma(U)=\int U(\xi)\sigma(d\xi)$.

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the above physical identifications have been made is deep and incompletely clarified. Note that the energy E may depend on physical parameters called "magnetic field," "chemical potential," etc. Note also that the traditional definition of the energy produces a minus sign in $\exp[-\beta E]$, which is in practice a nuisance. From now on we absorb β in the definition of U, and call U the *energy*. We shall retain from the above discussion only the hint that the Gibbs ensemble is an interesting object to consider in the limit of a "large system."

The thermodynamic formalism studies measures analogous to the Gibbs ensemble ρ in a certain limit where Ω becomes infinite, but some extra structure is present. Imitating the variational principle of the above Proposition, one defines *equilibrium states* (see II below). Imitating the definition (0.1), one defines *Gibbs states* (see III below).

II. Thermodynamic formalism on a metrizable compact set

Let Ω be a non-empty metrizable compact set, and $x \to \tau^x$ a homomorphism of the additive group $\mathbf{Z}^\nu$ ($\nu \geq 1$) into the group of homeomorphisms of Ω. We say that τ is *expansive* if, for some allowed metric d, there exists $\delta > 0$ such that

$$(d(\tau^x\xi, \tau^x\eta) \leq \delta \quad \text{for all } x) \quad \Rightarrow \quad (\xi = \eta).$$

Definition of the pressure. If $\mathfrak{A} = (\mathfrak{A}_i)$, $\mathfrak{B} = (\mathfrak{B}_j)$ are covers of Ω, the cover $\mathfrak{A} \vee \mathfrak{B}$ consists of the sets $\mathfrak{A}_i \cap \mathfrak{B}_j$. This notation extends to any finite family of covers. We write

$$\tau^{-x}\mathfrak{A} = (\tau^{-x}\mathfrak{A}_i),$$

$$\mathfrak{A}^\Lambda = \bigvee_{x \in \Lambda} \tau^{-x}\mathfrak{A} \qquad \text{if} \quad \Lambda \subset \mathbf{Z}^\nu,$$

$$\operatorname{diam} \mathfrak{A} = \sup_i \operatorname{diam} \mathfrak{A}_i,$$

where $\operatorname{diam} \mathfrak{A}_i$ is the diameter of $\mathfrak{A}_i$ for an allowed metric d on Ω.

The definition of the pressure which we shall now give will not look simple and natural to someone unfamiliar with the subject. This should not alarm the reader: the definition will give us quick access to a general statement of theorems of statistical mechanics. It will otherwise recur only in Chapter 6, with more preparation.

We denote by $\mathcal{C} = \mathcal{C}(\Omega)$ the space of continuous real functions on Ω. Let $A \in \mathcal{C}$, $\mathfrak{A}$ be a finite open cover of Ω, and Λ be a finite subset of $\mathbf{Z}^\nu$; define

$$Z_\Lambda(A, \mathfrak{A}) = \min\left\{ \sum_j \exp\left[\sup_{\xi \in \mathfrak{B}_j} \sum_{x \in \Lambda} A(\tau^x \xi) \right] \right.$$

$$\left. : (\mathfrak{B}_j) \text{ is a subcover of } \mathfrak{A}^\Lambda \right\}$$

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If $a^1,\ldots,a^\nu$ are integers >0, let $a=(a^1,\ldots,a^\nu)$ and

$$\Lambda(a)=\{(x^1,\ldots,x^\nu)\in\mathbf{Z}^\nu : 0\leqslant x^i<a^i \text{ for } i=1,\ldots,\nu\}.$$

The function $a\to\log Z_{\Lambda(a)}(A,\mathfrak{A})$ is subadditive, and one can write (with $|\Lambda(a)|=\operatorname{card}\Lambda(a)=\prod_i a^i$)

$$P(A,\mathfrak{A})=\lim_{a^1,\ldots,a^\nu\to\infty}\frac{1}{|\Lambda(a)|}\log Z_{\Lambda(a)}(A,\mathfrak{A})$$

$$=\inf_a \frac{1}{|\Lambda(a)|}\log Z_{\Lambda(a)}(A,\mathfrak{A}),$$

and

$$P(A)=\lim_{\operatorname{diam}\mathfrak{A}\to 0}P(A,\mathfrak{A}).$$

The function $P:\mathcal{C}\to\mathbf{R}\cup\{+\infty\}$ is the (topological) *pressure*. $P(A)$ is finite for all A if and only if $P(0)$ is finite; in that case P is convex and continuous (for the topology of uniform convergence in $\mathcal{C}$). $P(0)$ is the *topological entropy*; it gives a measure of the rate of mixing of the action τ.

Entropy of an invariant measure. If σ is a probability measure on Ω, and $\mathfrak{A}=(\mathfrak{A}_i)$ a finite Borel partition of Ω, we write

$$H(\sigma,\mathfrak{A})=-\sum_i \sigma(\mathfrak{A}_i)\log\sigma(\mathfrak{A}_i).$$

The real measures on Ω constitute the dual $\mathcal{C}^*$ of $\mathcal{C}$. The topology of weak dual of $\mathcal{C}$ on $\mathcal{C}^*$ is called the *vague* topology. Let $I\subset\mathcal{C}^*$ be the set of probability measures σ invariant under τ, i.e. such that $\sigma(A)=\sigma(A\circ\tau^x)$; I is convex and compact for the vague topology. If $\mathfrak{A}$ is a finite Borel partition and $\sigma\in I$, we write

$$h(\sigma,\mathfrak{A})=\lim_{a^1,\ldots,a^\nu\to\infty}\frac{1}{|\Lambda(a)|}H(\sigma,\mathfrak{A}^{\Lambda(a)})$$

$$=\inf_a\frac{1}{|\Lambda(a)|}H(\sigma,\mathfrak{A}^{\Lambda(a)});$$

$$h(\sigma)=\lim_{\operatorname{diam}\mathfrak{A}\to 0}h(\sigma,\mathfrak{A}).$$

The function $h:I\to\mathbf{R}\cup\{+\infty\}$ is affine $\geqslant 0$; it is called the (mean) *entropy*. If τ is expansive, h is finite and upper semi-continuous on I (with the vague topology).

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***Theorem* 1** (Variational principle).

$$P(A) = \sup_{\sigma \in I} \left[h(\sigma) + \sigma(A) \right]$$

for all $A \in C$.

This corresponds to the variational principle for finite systems if $-A$ is interpreted as the contribution to the energy of one lattice site.

Let us assume that P is finite. The set I_A of *equilibrium states* for $A \in \mathcal{C}$ is defined by

$$I_A = \{ \sigma \in I : h(\sigma) + \sigma(A) = P(A) \}.$$

I_A may be empty.

***Theorem* 2** *Assume that h is finite and upper semi-continuous on I (with the vague topology).*

(a) $I_A = \{ \sigma \in \mathcal{C}^* : P(A+B) \geq P(A) + \sigma(B)$ for all $B \in \mathcal{C} \}$. *This set is not empty; it is convex, compact; it is a Choquet simplex and a face of I.*
(b) *The set* $D = \{ A \in \mathcal{C} : \operatorname{card} I_A = 1 \}$ *is residual in* $\mathcal{C}$.
(c) *For every* $\sigma \in I$,

$$h(\sigma) = \inf_{A \in \mathcal{C}} \left[P(A) - \sigma(A) \right].$$

The fact that I_A is a metrizable simplex implies that each $\sigma \in I_A$ has a unique integral representation as the barycenter of a measure carried by the extremal points of I_A. It is known that I is also a simplex. The fact that I_A is a face of I implies that the extremal points of I_A are also extremal points of I (i.e. τ-ergodic measures on Ω).

III. Statistical mechanics on a lattice

The above theorems extend results known for certain systems of statistical mechanics (classical lattice systems). For instance, if F is a non-empty finite set (with the discrete topology), we can take $\Omega = F^{\mathbf{Z}^\nu}$ with the product topology, and τ^x defined in the obvious manner. More generally we shall take for Ω a closed τ-invariant non-empty subset of $F^{\mathbf{Z}^\nu}$. For the physical interpretation, note that Ω is the space of infinite configurations of a system of spins on a crystal lattice $\mathbf{Z}^\nu$. Up to sign and factors of β, P can be interpreted as the "free energy" or the "pressure," depending on the physical interpretation of F as the set of "spin values" or of "occupation numbers" at a lattice site. For simplicity we have retained the word "pressure."

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